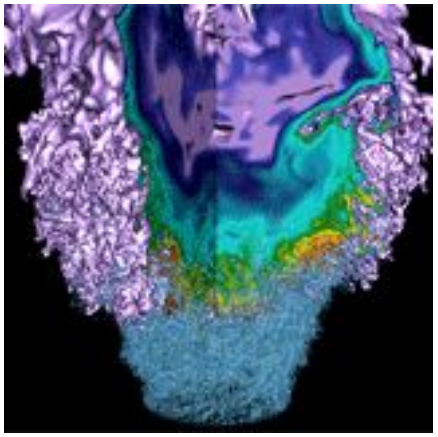
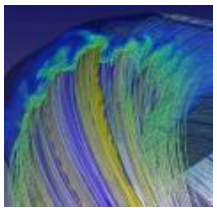
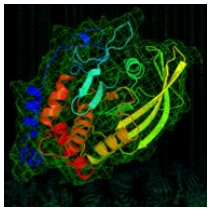
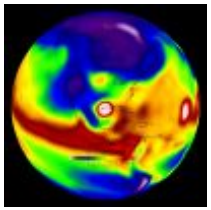
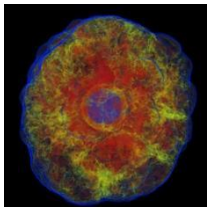
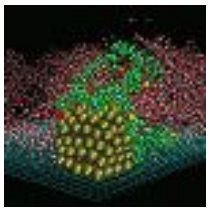
Data Management, I/O Libraries and Databases at NERSC



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U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB

Outline

- Data Management Best Practices and Guidelines
- I/O Libraries
- Databases

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- **Data Management Best Practices and Guidelines**
- I/O Libraries
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Why Manage Your Data?

- **"Data management is the development, execution and supervision of plans, policies, programs and practices that control, protect, deliver and enhance the value of data and information assets."***

*DAMA-DMBOK Guide (Data Management Body of Knowledge) Introduction & Project Status

Data @ NERSC

NERSC offers a variety of services to support data-centric workloads. We provide tools in the areas of:

- **Data Analytics (statistics, machine learning, imaging)**
- **Data Management (storage, representation)**
- **Data Transfer**
- **Workflows**
- **Science Gateways**
- **Visualization**

http://www.nersc.gov/users/data-analytics/

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General Recommendations

- **NERSC recommends the use of modern, scientific I/O libraries (HDF5, netCDF, ROOT) to represent and store scientific data.**
- **We provide database technologies (MongoDB, SciDB, MySQL, PostGreSQL) for our users as a complementary mechanism for storing and accessing data.**
- **Low-level, POSIX I/O from applications to NERSC file systems, if necessary. Details here:**

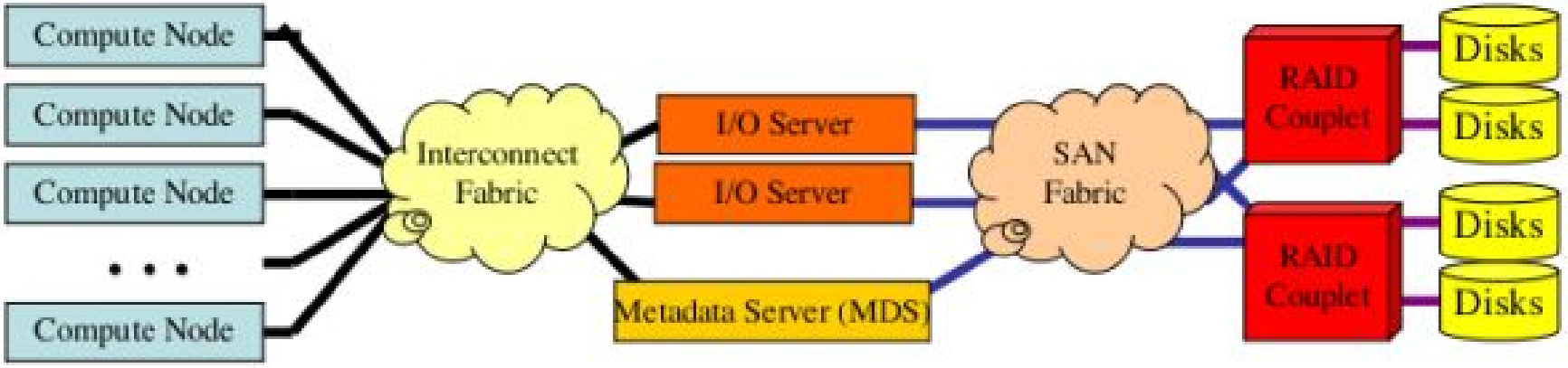
  http://www.nersc.gov/users/storage-and-file-systems/

Notes on NERSC File I/O

- **Use the local scratch file system on Edison and Cori for best I/O rates.**
- **For some types of I/O you can further optimize I/O rates using a technique called file striping.**
- **Keep in mind that data in the local scratch directories are purged, so you should always backup important files to HPSS* or project space.**
- **You can share data with your collaborators using project directories. These are directories that are shared by all members of a NERSC repository.**

*HPSS: http://www.nersc.gov/users/storage-and-file-systems/hpss/getting-started/

Lustre



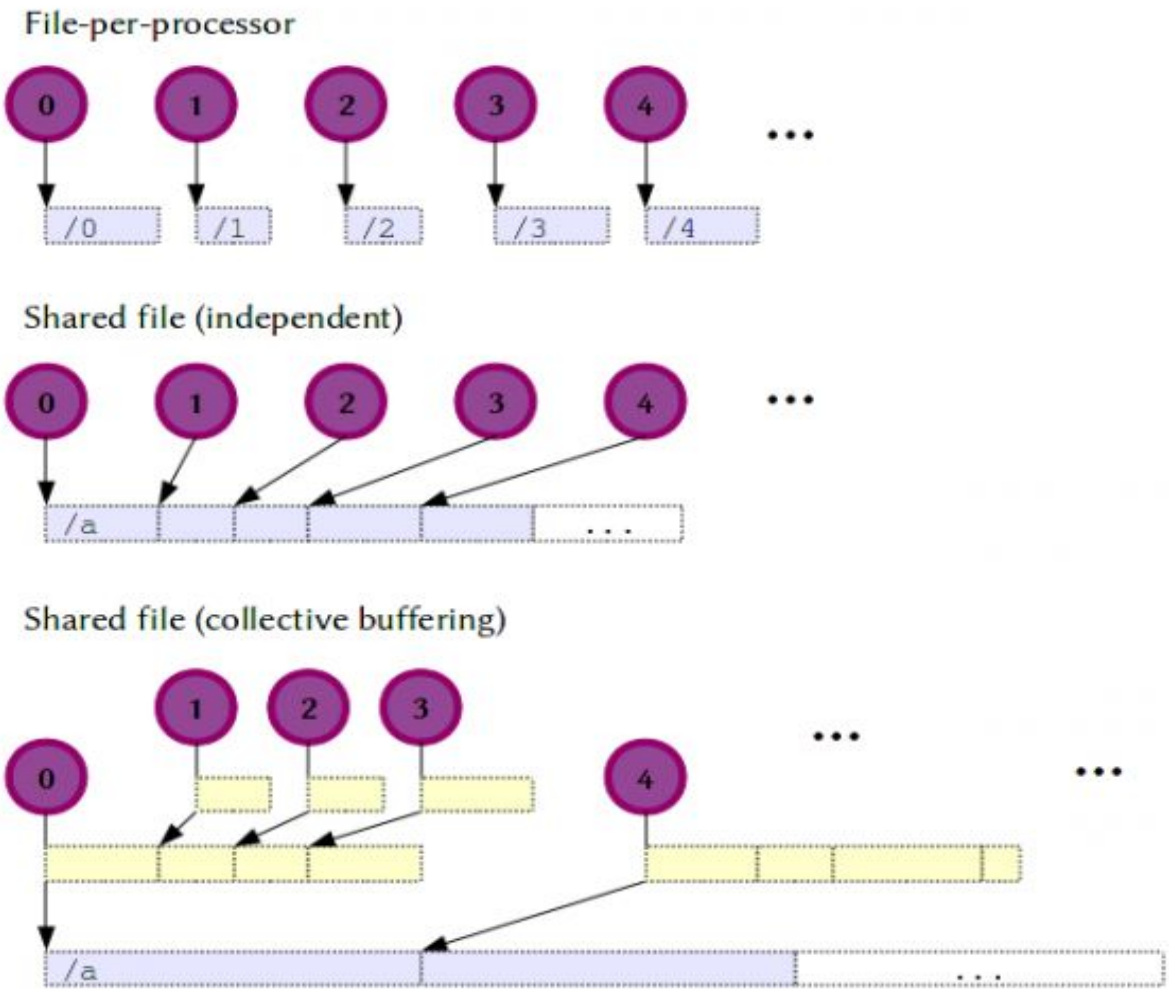
- **Scalable, POSIX-compliant parallel file system designed for large, distributed-memory systems**
- **Uses a client-server model with separate servers for file metadata and file content**

Scientific I/O

I/O is commonly used by scientific applications to achieve goals like:

- **Storing numerical output from simulations for later analysis or workflow stages**
- **Implementing 'out-of-core' techniques for algorithms that process more data than can fit in system memory and must page in data from disk**
- **Checkpointing application state to files, in case of application or system failure.**

Types of Application I/O to Parallel File Systems



MPI Collective I/O

- ***Collective I/O*** **refers to a set of optimizations available in many implementations of MPI-IO that improve the performance of large-scale IO to shared files.**
- **To enable these optimizations, you must use the *collective* calls in the MPI-IO library that end in *_all***
  - For instance: MPI_File_write_at_all().
- **And, all MPI tasks in the given MPI communicator must participate in the collective call, even if they are not performing any IO operations.**
- **The MPI-IO library has a heuristic to determine whether to enable *collective buffering*, the primary optimization used in collective mode.**

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Why I/O Middleware?

- **The complexity of I/O systems poses significant challenges in investigating the root cause of performance loss.**
- **Use of I/O middleware for writing parallel applications can greatly enhance application developer productivity.**
  - Such an approach hides many of the complexities associated with performing parallel I/O, rather than relying purely on programming language aids and parallel library support, such as MPI.

I/O Middleware @ NERSC

- **HDF5**
  - A data model and set of libraries & tools for storing and managing large scientific datasets.
- **netCDF**
  - A set of libraries and machine-independent data formats for creation, access, and sharing of array-oriented scientific data.
- **ROOT**
  - A self-describing, column-based binary file format that allows serialization of a large collection of C++ objects and efficient subsequent analysis.
- **Others**
  - http://www.nersc.gov/users/data-analytics/data-management/i-o-libraries/i-o-library-list/

HDF5

- **The Hierarchical Data Format v5 (HDF5) library is a portable I/O library used for storing scientific data.**
- **The HDF5 technology suite includes:**
  - A versatile data model that can represent very complex data objects and a wide variety of metadata.
  - A completely portable file format with no limit on the number or size of data objects in the collection.
  - A software library that runs on a range of computational platforms, from laptops to massively parallel systems, and implements a high-level API with C, C++, Fortran 90, and Java interfaces.
  - A rich set of integrated performance features that allow for access time and storage space optimizations.
  - Tools and applications for managing, manipulating, viewing, and analyzing the data in the collection.
- **HDF5's 'object database' data model enables users to focus on high-level concepts of relationships between data objects rather than descending into the details of the specific layout of every byte in the data file.**

netCDF

- **netCDF ("Network Common Data Form") is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.**
- **netCDF is:**
  - Typically used in the climate field
  - More constrained than HDF5
  - At a higher level of abstraction
- **More netCDF information here:**

  http://www.unidata.ucar.edu/software/netcdf/docs/netcdf/

ROOT

- **A set of object oriented frameworks with the functionality needed to handle and analyze large amounts of data in an efficient way.**
  - Heavily used in experimental HEP/NP
- **ROOT is written in C++ and creates self-describing files, with a flexible object serialization and fast column-oriented access.**
- **Originally designed for particle physics, its usage has extended to other data-intensive fields like astrophysics and neuroscience.**
  - Integrated histogramming / querying/ machine learning and in most HEP experiment frameworks.
  - ROOT is mainly used for data analysis at NERSC.
- **ROOT Docs: https://root.cern.ch/drupal/**

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Databases @ NERSC

- **NERSC supports the provisioning of databases to hold large scientific datasets, as part of the science gateways effort.**
- **Data-centric science often benefits from database solutions to store scientific data or metadata about data stored in more traditional file formats like HDF5, netCDF or ROOT.**
- **Our database offerings are targeted toward large data sets and high performance. Currently we support:**
  - MySQL
  - PostgreSQL
  - MongoDB
  - SciDB
- **If you would like to request a database at NERSC please fill out this form and you'll be contacted by NERSC staff: http://www.nersc.gov/users/data-analytics/data-management/databases/science-database-request-form/**

PostgreSQL

- **PostgreSQL is an object-relational database. It is known for having powerful and advanced features and extensions as well as supporting SQL standards.**
- **NERSC provides a set of database nodes for users that wish to use PostgreSQL with their scientific applications.**
- **PostgreSQL documentation here:**

  http://www.postgresql.org/docs/

MySQL

- **MySQL is a very popular and powerful open-source relational database.**
- **Many features:**
  - Pluggable Storage Engine Architecture, with multiple storage engines:
    - InnoDB
    - MyISAM
    - NDB (MySQL Cluster)
    - Memory
    - Merge
    - Archive
    - CSV
    - and more
  - Replication to improve application performance and scalability
  - Partitioning to improve performance and management of large database applications
  - Stored Procedures to improve developer productivity
  - Views to ensure sensitive information is not compromised
  - …
- **MySQL user documentation:**
  http://dev.mysql.com/doc/

SciDB

- **SciDB is a parallel database for array-structured data, good for TBs of time series, spectra, imaging, etc.**
- **A full ACID database management system that stores data in multidimensional arrays with strongly-typed attributes (aka fields) within each cell.**
- **SciDB User Documentation:**

  https://paradigm4.atlassian.net/wiki/display/ESD/SciDB+Documentation
- **To request access to NERSC SciDB instances, please email consult@nersc.gov**

MongoDB

- **A cross-platform document-oriented database.**
- **Classified as a *NoSQL* database, MongoDB eschews the traditional table-based relational database structure in favor of JSON-like documents with dynamic schemas, making the integration of data in certain types of applications easier and faster.**
- **MongoDB user documentation:**

  https://docs.mongodb.com/v2.6/

Questions, Comments, Feedback?